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Sent: Monday, January 09, 2006 12:33 PM
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A method for calculating a potential of mean force (PMF) score of a protein-ligand complex, the method comprising:
accessing one or more parameters useable to calculate a repulsion term useable to calculate a PMF of a protein-ligand atom pair in the protein-ligand complex, the one or more parameters corresponding to an atom-pair type of the protein-ligand atom pair;
using the one or more accessed parameters, calculating the repulsion term useable to calculate the PMF of the protein-ligand atom pair; and
communicating the calculated repulsion term for calculation of the PMF score of the protein-ligand complex.

Key terms: potential of mean force (PMF); repulsion; parameter; protein; ligand

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Filing date: 9/5/2003

Paper printout please
Thanks, MKZ

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